Washington University in St. Louis
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Topics in Quantum Mechanics

Chemistry

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First Order Time Evolution

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A Simple Mechanical System with First Order Time Evolution

A. The Simple Harmonic Oscillator

The equation of motion for a simple one-dimensional harmonic oscillator,

$$\ddot{x}(t) + \omega^2 x(t) = 0,$$

can be written as two (coupled) first order equations,

$$\dot{x}(t) = v(t),$$
$$\dot{v}(t) = -\,\omega^2 x(t).$$

B. Replace $\{x(t), v(t)\} \rightarrow z(t)$

If

$$z(t) = x(t) + i\frac{v(t)}{\omega},$$

with $i^2 = -1$,

$$\dot{z}(t) = \dot{x}(t) + i\frac{\dot{v}(t)}{\omega} = v(t) - i\,\omega\,x(t) = -i\,\omega\left[x(t) + i\frac{v(t)}{\omega}\right] = -i\,\omega\,z(t)$$

The second order (in time) equation for $x(t)$ has been replaced by a first order (in time) equation for $z(t)$.

C. The simpler equation of motion is easer to solve

Reducing the dynamical equation to

$$\dot{z}(t) = -i\,\omega\,z(t) \tag{1}$$

produces a *simpler* mathematical task. If the subscript $_0$ labels initial conditions, the solution of Eq(1) is

$$z(t) = e^{-i\omega\,t} z_0 \tag{2}$$

D. Go back to $x(t)$ and $v(t)$

In terms of $x(t)$ and $v(t)$, Eq.(2) reads

$$x(t) + i\frac{v(t)}{\omega} = e^{-i\omega\, t}\left[x_0 + i\frac{v_0}{\omega}\right] = [\cos(\omega\, t) - i\,\sin(\omega\, t)]\left[x_0 + i\frac{v_0}{\omega}\right]$$

Separting the real and imaginary components of this identifies

$$\begin{aligned} x(t) =& x_0\,\cos(\omega\, t) + \frac{v_0}{\omega}\sin(\omega\, t) \\ v(t) =& v_0\,\cos(\omega\, t) - \omega\, x_0\,\sin(\omega\, t) \end{aligned}$$

the correct solution to the simple harmonic oscillator dynamical problem.